Nuclear Schiff moment and soft vibrational modes

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The atomic electric dipole moment (EDM) currently searched by a number of experimental groups requires that both parity and time-reversal invariance be violated. According to current theoretical understanding, the EDM is induced by the nuclear Schiff moment. The enhancement of the Schiff moment by the combination of static quadrupole and octupole deformation was predicted earlier. Here we study a further idea of the possible enhancement in the absence of static deformation but in a nuclear system with soft collective vibrations of two types. Both analytical approximation and numerical solution of the simplified problem confirm the presence of the enhancement. We discuss related aspects of nuclear structure which should be studied beyond mean-field and random phase approximations.

I. INTRODUCTION

Efforts of many experimental groups are directed to the discovery of the *electric dipole moment* (EDM) of atoms. The existence of the EDM in a stationary state of a finite quantum system would manifest the *simultaneous violation* of parity ($\mathcal{P}$-) and time-reversal ($\mathcal{T}$-) invariance [1]. The best current experimental limits [2, 3] are found for ^{129}Xe and ^{199}Hg. Further progress in this field can be connected with the better understanding of nuclear many-body mechanisms which could substantially enhance the effect. This problem is also of significant interest for theory of collective motion in nuclei and other mesoscopic systems.

The atomic dipole moment is induced by the weak interactions of atomic electrons with the nucleus. The dipole moment of the nucleus is almost completely screened by the redistribution of atomic electrons in the applied external electric field (the famous *Schiff theorem* [4]). Instead of the nuclear dipole moment, one needs to consider the vector operator of the next order, the so-called *Schiff moment* [5],

$$\mathbf{S} = \frac{1}{10}\sum_a e_a \mathbf{r}_a \left[r_a^2 - \frac{5}{3}\langle r_{\rm ch}^2\rangle \right]. \tag{1}$$

The correctness of this conclusion was confirmed in the recent theoretical discussion that lead to the reexamination of the Schiff theorem [6, 7]. The similar operator is known as generating the isoscalar giant dipole resonance in nuclei since the isoscalar dipole moment creates only a spurious mode of the center-of-mass displacement.

In the presence of $\mathcal{P},\mathcal{T}$-violating weak interaction, the non-zero expectation value of the Schiff moment, as of any polar time-even vector, becomes possible in the ground state of a nucleus with non-zero angular momentum I,

$$\langle \mathbf{S}\rangle = \langle (\mathbf{S}\cdot\mathbf{I})\rangle \, \frac{\mathbf{I}}{I(I+1)}. \tag{2}$$

In the next step, this vector induces the EDM of the atom that is enhanced in heavy atoms. Typically, the Schiff moment has a single-particle order of magnitude value as confirmed by various calculations of nuclear structure, see for example [8, 9, 10, 11]; the core polarization effects can increase the result by a factor of order 2.

It is however known that there exist promising collective mechanisms which must be explored in the search of the many-body enhancement of the Schiff moment. Parity non-conservation in scattering of polarized neutrons off heavy nuclei is enhanced by orders of magnitude [12] because of extreme proximity of p- and s-wave resonances and the *chaotic nature* of their extremely complicated wave functions. In contrast, here we are interested in *coherent* mechanisms which could show up in the properties of the ground states and low-lying excitations. Essentially we need the collective states of opposite parity in the vicinity of the ground state which can be effectively admixed to the ground state by the weak interaction. The main hope here is associated with *coexistence of quadrupole and octupole collective degrees of freedom*. Indeed, it was shown that the *intrinsic* Schiff moment (in the body-fixed frame), that exists without violation of fundamental symmetries, can be enhanced by 2-3 orders of magnitude in nuclei with simultaneous quadrupole and octupole static deformation [13, 14, 15]. The mixing by the weak interaction of states with certain angular momentum in the laboratory (space-fixed) frame will be particularly enhanced for *parity doublets* [16, 17, 18]. Those are the states with same spin and opposite parity which differ by the “right” and “left”

orientation of the asymmetric configuration that is characteristic for the deformation without reflection symmetry in the equatorial plane.

The requirements of static octupole deformation can be relaxed since almost the same effect can be reached [18, 19] when static quadrupole deformation is combined with a soft octupole vibrational mode. Similarly to the case of static octupole deformation, where the enhancement effect is proportional to the square β_3^2 of the octupole deformation parameter, here the analogous result contains the dynamic mean square value $\langle\beta_3^2\rangle$ that has the same order of magnitude being proportional to the inverse soft mode frequency, $1/\omega_3$. This significantly widens the set of nuclear candidates where one can expect the collective enhancement of the Schiff moment.

There is a theoretical possibility that the enhancement may occur even in the absence of static quadrupole deformation due to the combination of *quadrupole and octupole soft modes* [20, 21]. This would broaden even further the possibilities for the experimental search of the EDM adding, for example, such nuclei as light isotopes of radium and radon, where the presence of both soft modes with strong dipole transitions connecting corresponding vibrational bands is well known [22]. Although phenomenological estimates [20] supported this idea, the detailed microscopic calculation [21] based on the random phase approximation (RPA) and quasiparticle-phonon coupling gave essentially negative results. The effect of strong enhancement was found only in the unphysical limit of very low vibrational frequencies ω_2 and ω_3. However, the applicability of the RPA to the situation of strong interaction of low-frequency collective modes is questionable and that result might be an artifact of the inappropriate approximation.

In the current work we present a simplified model, where an unpaired particle interacts with two coupled soft collective modes. This interaction is effectively strong and creates a *coherent state (condensate) of phonons* although the even core is still spherical. Such a situation cannot be adequately treated in the RPA framework. We consider both the approximate analytical approach and exact numerical solution. The results clearly demonstrate the existence of a parameter region, where we see the strong enhancement of the nuclear Schiff moment. On the other hand, the whole problem is quite interesting irrespectively of the symmetry violations, for the study of nuclear structure in the situation of shape instability due to the presence of soft modes. A more detailed review of the entire problem of the Schiff moment and the previous search for its collective enhancement can be found in [23].

II. MICROSCOPIC JUSTIFICATION OF ENHANCEMENT

A. Spontaneous symmetry breaking in an even nucleus with soft modes

We consider a generic model of a "soft" nucleus that has well developed vibrational modes still keeping, on average, a spherical shape. Although the non-zero Schiff moment requires non-zero nuclear spin and therefore an odd-A nucleus, we start with the neighboring even-even nuclei. Here we assume that the collective modes with spin-parity characteristics 2^+ and 3^- have low excitation energies ω_2 and ω_3, well below the gap energy 2Δ that separates the ground state 0^+ from the threshold of two-quasiparticle states. This situation, for example, can be found in the chain of even-even xenon isotopes [24] and, most clearly, in light isotopes of radon and radium [22], where we see soft quadrupole and octupole collective modes evidently correlated in their energetics. As the energy spectrum does not display a rotational pattern, we can assume that these nuclei are still spherical. However, the spectra do not show usual phonon multiplets either. In radium and radon isotopes, strong dipole transitions are present between the corresponding members of long quasivibrational bands of positive and negative parity. This situation seems to be favorable for dipole correlations, and consequently for the Schiff moment.

The correlation between quadrupole and octupole vibrations is an anharmonic effect that can be theoretically described only if one goes beyond the random phase approximation (RPA). In the following part of the article, Sec. III, we show a numerically solved two-level model that starts from single-particle mean field levels and an inter-particle interaction; then both phonons and anharmonic effects result from the exact diagonalization. In the present Section we use a simpler analytical approximation of bosonic phonons interacting with unpaired particles. The model is a generalization of the approach suggested in Ref. [25] for a global analysis of quadrupole-octupole correlations. This idea was later used for the explanation of such correlations seen in the experimental data for xenon isotopes [24] and in the schematic arguments applied to the ehnancement of the Schiff moment in Ref. [21]. The correlations between quadrupole and octupole modes can lead to new observable effects and phase transitions also in nuclei with $A > 220$ as it was discussed recently [26, 27].

The model includes two groups of spherical single-particle levels with spins $\{j\}$ and $\{j'\}$ of positive and negative parity, respectively. The elementary bosonic quanta, phonons, are coherent superpositions of many two-quasiparticle excitations. The quadrupole phonons d_μ contain $(j_1 j_2)_{2\mu}$ and $(j'_1 j'_2)_{2\mu}$ combinations allowed by the angular momentum coupling, while the octupole phonons f_μ are built of the pairs $(j_1 j'_2)_{3\mu}$ based on the orbitals of opposite parity. The

effective Hamiltonian of low-lying states in the even nucleus is given by

$$H = H_2 + H_3 + H_{23}, \tag{3}$$

where H_2 and H_3 describe quadrupole and octupole collective modes (in principle including their anharmonicity). The interaction term,

$$H_{23} = x \sum_{\mu} \Big[(f^\dagger f)_{2\mu} d^\dagger_\mu + \text{h.c.} \Big], \tag{4}$$

is responsible for the mode-mode interaction with x as a coupling constant. The construction of (4) is the simplest one that accounts for parity and angular momentum conservation.

The non-linear interaction (4) leads to the effective deformation of the excited states when both modes are simultaneously present. Indeed, the low-lying quadrupole and octupole modes support each other and generate the *coherent state* with the non-vanishing expectation value of the quadrupole moment according to

$$\langle d_\mu \rangle = -\frac{x}{\omega_2} \langle (f^\dagger f)_{2\mu} \rangle, \tag{5}$$

as follows from the operator equation of motion

$$[d_\mu, H] = \omega_2 d_\mu + x (f^\dagger f)_{2\mu}. \tag{6}$$

for the quadrupole phonon operator d_μ. For simplicity, here we neglect the possible quadrupole anharmonicity that would only substitute the unperturbed quadrupole frequency ω_2 by the effective curvature of the ground state quadrupole potential [28].

The result (5) means *spontaneous violation of rotational symmetry* by the soft quadrupole mode that is determined by the octupole phonon which selects the intrinsic axis (we assume axial symmetry). The direction of the effective self-consistent deformation is arbitrary, and, to restore the symmetry and appropriate quantum numbers of total nuclear spin in the space-fixed coordinate frame, we accept that the orientation of the deformation is given by a spherical function of corresponding rank,

$$\langle d_\mu \rangle = \delta_2 \sqrt{\frac{4\pi}{5}}\, Y^*_{2\mu}(\mathbf{n}), \quad \langle f_\mu \rangle = \hat{f} \sqrt{\frac{4\pi}{7}}\, Y^*_{3\mu}(\mathbf{n}). \tag{7}$$

Here $\mathbf{n}$ is the unit vector of the symmetry axis considered as a variable in the collective space. A similar operator approach was used long ago in the derivation of the nuclear moment of inertia without applying a cranking model [29].

The number $N_3 = \sum_\mu f^\dagger_\mu f_\mu = \hat{f}^\dagger \hat{f}$ of octupole phonons is conserved, $N_3 = 1$ in the lowest 3^- state, and $\hat{f}^\dagger$ is the operator generating the octupole vibrational mode in the body-fixed frame defined by the orientation $\mathbf{n}$. Then eq. (5) equates the $\mathbf{n}$-dependence and, with the ansatz (7), provides the effective quadrupole deformation parameter δ_2,

$$\delta_2 = -\frac{x}{\omega_2} \sqrt{5} \begin{pmatrix} 3 & 3 & 2 \\ 0 & 0 & 0 \end{pmatrix} = -\sqrt{\frac{4}{21}}\, \frac{x}{\omega_2}. \tag{8}$$

The $1/\omega$-dependence of the effective deformation parameters is the characteristic feature of the whole consideration based on the assumption of soft collective modes.

The equation of motion for the octupole mode, given by the commutator $[f_\mu, H]$ and the effective quadrupole parameter (8), is linear. It relates the excitation energy E_3 of the octupole phonon with the corresponding unperturbed energy ω_3 and the quadrupole condensate (8). Collecting again the terms expressing the angular dependence, we obtain

$$E_3 = \omega_3 - \frac{8}{21} \frac{x^2}{\omega_2}. \tag{9}$$

This simple regularity first discussed in Ref. [25] in the global review of octupole vibrations provides a clear correlation between the two modes. Recent measurements for the long chain of even-even xenon isotopes [24] show precisely such a correlation, with a rather large magnitude for the parameter x that exceeds the expectations for the anharmonic mode-mode coupling based on the standard RPA estimates. We assume that the Schiff vector $\mathbf{S}$ has a non-zero reduced matrix element S° between the one-phonon states of the two modes, $|2^+\rangle$ and $|3^-\rangle$.

B. Phonon condensate in an odd nucleus

Now we consider the situation in the adjacent odd-A nucleus, where the presence of the unpaired particle in the ground state breaks symmetry for both soft modes. The state of the odd particle is defined by the density matrix

$$\rho_{j_1m_1;j_2m_2} = a^{\dagger}_{j_2m_2}a_{j_1m_1} \tag{10}$$

in terms of the operators of creation, $a^{\dagger}_{jm}$, and annihilation, a_{jm}, of the particle. The expectation value $\langle\rho_{j_1m_1;j_2m_2}\rangle$ in the ground state with spontaneously broken symmetry can be written as

$$\langle\rho_{j_1m_1;j_2m_2}\rangle = \sum_{L\Lambda}(-)^{L-\Lambda+j_2-m_2}\begin{pmatrix} j_1 & L & j_2 \\ m_1 & -\Lambda & -m_2 \end{pmatrix}\rho_L(j_1j_2)Y^*_{L\Lambda}(\mathbf{n}). \tag{11}$$

Here the even-L parts come from the pairs of levels (j_1, j_2) or (j'_1, j'_2) of the same parity, whereas the odd-L ones correspond to the combinations (j_1, j'_2) and (j'_1, j_2) of single-particle levels of opposite parity.

In the odd nucleus, the unpaired particle interacts with the soft modes, and the phonon Hamiltonian should be supplemented with

$$H_{\rm odd} = h + H^{(+)} + H'^{(+)} + H^{(-)}, \tag{12}$$

where h contains unperturbed spherical single-particle energies ϵ_j and $\epsilon_{j'}$, or quasiparticle energies if pairing is included. The positive-parity parts are given by

$$H^{(+)} = -\sum_{j_1j_2m_1m_2\mu} x^{(+)}_{j_1j_2}\rho_{j_1m_1;j_2m_2}$$

$$\times\left(d^{\dagger}_{\mu} + (-)^{\mu}d_{-\mu}\right)(-)^{\mu+j_2-m_2}\begin{pmatrix} j_1 & 2 & j_2 \\ m_1 & -\mu & -m_2 \end{pmatrix}, \tag{13}$$

and $H'^{(+)}$, where all positive parity levels j are substituted by the negative parity levels j'. The Hermiticity conditions for the Hamiltonian (11) and its negative-parity analog read

$$x^{(+)}_{j_1j_2} = (-)^{j_1-j_2}(x^{(+)}_{j_2j_1})^*, \quad {x'}^{(+)}_{j'_1j'_2} = (-)^{j'_1-j'_2}({x'}^{(+)}_{j'_2j'_1})^*. \tag{14}$$

The interaction with the octupole phonon that changes parity of the particle is, analogously,

$$H^{(-)} = -\sum_{j_1j'_2m_1m_2\mu} y_{j_1j'_2}\rho_{j_1m_1;j'_2m_2}$$

$$\times\left(f^{\dagger}_{\mu} + (-)^{\mu}f_{-\mu}\right)(-)^{\mu+j'_2-m_2}\begin{pmatrix} j_1 & 3 & j'_2 \\ m_1 & -\mu & -m_2 \end{pmatrix} + \text{h.c.}, \tag{15}$$

Here we take the coordinate part of the phonon field, for example, $(d^{\dagger}_{\mu} + (-)^{\mu}d_{-\mu}\Big)$, since it is proportional to $1/\sqrt{\omega}$ in contrast to the momentum part (with sign minus between the phonon creation and annihilation operators) that is small, $\propto \sqrt{\omega}$, for a soft mode.

With the directions specified by the unpaired particle, the soft modes acquire the condensate components in the ground state of the odd nucleus. In the same way as shown by eq. (7) we find

$$\langle d_{\mu}\rangle = \beta_2Y^*_{2\mu}(\mathbf{n}) = \frac{1}{5\omega_2}\left[\sum_{j_1j_2}x^{(+)}_{j_1j_2}\rho_2(j_1j_2) + \sum_{j'_1j'_2}{x'}^{(+)}_{j'_1j'_2}\rho_2(j'_1j'_2)\right]Y^*_{2\mu}(\mathbf{n}), \tag{16}$$

$$\langle f_{\mu}\rangle = \beta_3Y^*_{3\mu}(\mathbf{n}) = \frac{1}{7\omega_3}\left[\sum_{j_1j'_2}y_{j_1j'_2}\rho_3(j_1j'_2) + \sum_{j'_1j_2}y_{j'_1j_2}\rho_3(j'_1j_2)\right]Y^*_{3\mu}(\mathbf{n}). \tag{17}$$

C. Density matrix of an unpaired particle

The presence of phonon condensates self-consistently creates effective deformation of the mean field for an unpaired particle. This is revealed in the appearance of deformed components $\rho_{L\neq 0}$ of the density matrix (11). The equations of motion for the single-particle operators can be written as

$$[a_{jm},H] = \epsilon_j a_{jm} - \sum_{j_1 m_1 \mu} x^{(+)}_{j_1 j}\Big(d^\dagger_\mu + (-)^\mu d_{-\mu}\Big)(-)^{\mu+j-m}\begin{pmatrix} j_1 & 2 & j \\ m_1 & -\mu & m\end{pmatrix} a_{j_1 m_1}$$

$$- \sum_{j_1' m_1 \mu} y_{j_1' j}\Big(f^\dagger_\mu + (-)^\mu f_{-\mu}\Big)(-)^{\mu+j-m}\begin{pmatrix} j_1' & 3 & j \\ m_1 & -\mu & m\end{pmatrix} a_{j_1' m_1}. \tag{18}$$

A similar equation is valid for the operators $a_{j'm}$ related to the negative parity levels with obvious substitutions $x^{(+)} \to x'^{(+)}$ and $y_{j_1' j} \to y_{j j_1'}$.

As now the odd particle is moving in the mean field of effective deformation, its angular momentum j is not conserved anymore but, owing to the assumed axial symmetry, the angular momentum projection κ onto the symmetry axis still characterizes the single-particle levels. The appropriate transformation for the single-particle operators is therefore

$$a_{jm} = \sum_\kappa D^j_{m\kappa} c_{j\kappa}, \tag{19}$$

where we use the matrix elements $D^j_{m\kappa}$ of finite rotations. Such angular functions, after straightforward algebra, appear in all terms of equations of motion (18) justifying the ansatz (19). The new operators $c_{j\kappa}$ satisfy, instead of (19), the set of equations

$$[c_{j\kappa},H] = \epsilon_j c_{j\kappa} - 2\beta_2\sqrt{\frac{5}{4\pi}}\sum_{j_1} x^{(+)}_{j_1 j}(-)^{j_1-\kappa}\begin{pmatrix} j_1 & 2 & j \\ -\kappa & 0 & \kappa\end{pmatrix} c_{j_1\kappa}$$

$$- 2\beta_3\sqrt{\frac{7}{4\pi}}\sum_{j_1'} y_{j_1' j}(-)^{j_1'-\kappa}\begin{pmatrix} j_1 & 3 & j \\ -\kappa & 0 & \kappa\end{pmatrix} c_{j_1'\kappa}, \tag{20}$$

and analogously for the operators $c_{j'\kappa}$ for the levels originally of negative parity. In the intrinsic frame parity is mixed by the simultaneous presence of quadrupole and octupole deformation [we used in eq. (20) the static values (16) and (17)]. These coupled equations provide deformed single-particle states and their energy spectrum. For the states with one unpaired particle, the transformation (19) is normalized as

$$\sum_{jm}\langle a^\dagger_{jm} a_{jm}\rangle = \sum_{j\kappa}\langle c^\dagger_{j\kappa} c_{j\kappa}\rangle = 1. \tag{21}$$

When the linear set of equations (20) is solved and the Nilsson-type single-particle orbitals with no definite parity are found, we can return to the density matrix (11) and make the consideration self-consistent. From eq. (11) we obtain

$$\rho_L(j_1 j_2) = \sqrt{4\pi(2L+1)}(-)^L\sum_\kappa (-)^{j_2-\kappa}\begin{pmatrix} j_2 & j_1 & L \\ -\kappa & \kappa & 0\end{pmatrix}\langle c^\dagger_{j_2\kappa} c_{j_1\kappa}\rangle. \tag{22}$$

A similar expression is valid for $\rho_L(j_1' j_2')$ and for the mixed-parity components of the density matrix $\rho_L(j_1 j_2')$.

D. Schiff moment

The operator $S_{1\nu}$ of the Schiff moment in the even nucleus has a reduced matrix element $S^\circ \equiv (2||S_1||3)$ between the low-lying 2^+ and 3^- states. As mentioned earlier, the dipole transitions between the states of the quadrupole and octupole bands are empirically known to be enhanced in nuclei of our interest, such as light radium and radon isotopes [22]. The collective contribution to this operator can be written in terms of our phonon variables as

$$S_{1\nu} = S^\circ \sum_{\mu\mu'}(-)^{\nu+\mu}\begin{pmatrix} 1 & 2 & 3 \\ -\nu & -\mu & \mu'\end{pmatrix}\Big(d^\dagger_\mu f_{\mu'} + (-)^{\mu+\mu'} f^\dagger_{-\mu'} d_{-\mu}\Big). \tag{23}$$

With the ground state expectation values of the effective deformation parameters in the odd nucleus, eqs. (16) and (17), this gives a rotational operator

$$\frac{S_{1\nu}}{S^{\circ}} = -\frac{1}{\sqrt{\pi}}\,\beta_2\beta_3 Y^{*}_{1\nu} \tag{24}$$

enhanced by small collective frequencies. As a result, we reduce the whole problem to that of the "particle + rotor" type [14, 30], where the static deformation is substituted by the effective deformation coming from the soft quadrupole and octupole modes of the spherical even core.

The observable Schiff moment in the laboratory frame can come only from the explicitly acting $\mathcal{P}$- and $\mathcal{T}$-violating weak interaction W that creates an admixture of the states $|n\rangle$ of opposite parity to the ground state $|0\rangle$,

$$\langle \mathbf{S}\rangle = \sum_{n} \frac{W_{0n}\mathbf{S}_{n0} + \mathbf{S}_{0n}W_{n0}}{E_0 - E_n}. \tag{25}$$

The states $|n\rangle$ must have the same spin $I \neq 0$ as the ground state of the odd nucleus since W is a rotational scalar.

E. Simple model

The structure of equations becomes clear in the simple model case of two levels j and j' of opposite parity but the same magnitude $j = j'$. The single-particle spherical energy levels are ϵ and ϵ', while the corresponding single-particle operators in the intrinsic frame are c_κ and c'_κ, where κ is the projection of the single-particle angular momentum onto the symmetry axis. The analysis essentially follows the consideration [14] developed for a statically deformed nucleus with no symmetry with respect to the reflection in the equatorial plane.

The effectively deformed core is presented by rotational states $(D^L_{M'0})^* = \sqrt{4\pi/2L+1}\,Y_{LM'}$, where parity is simply $(-)^L$. The particle orbitals are defined by the operators $c^\dagger_\kappa$ for positive parity and ${c'_\kappa}^\dagger$ for negative parity multiplied by the corresponding rotational functions $D^j_{m\kappa}$ which are coupled with the core D^L-functions to the total angular momentum I and laboratory projection M of the nucleus (the body-fixed projection is $K = \kappa$). Due to the presence of octupole deformation, the intrinsic particle states $|\kappa\rangle$ do not have certain parity. Their wave functions can be written as

$$|\kappa) = (\xi_\kappa c^\dagger_\kappa + \eta_\kappa {c'_\kappa}^\dagger)|0\rangle, \quad \xi^2_\kappa + \eta^2_\kappa = 1, \tag{26}$$

and the amplitudes ξ_κ and η_κ satisfy the secular equations with split energies E_κ,

$$[E_\kappa - \epsilon + b_2(\kappa)]\xi_\kappa + b_3(\kappa)\eta_\kappa = 0, \tag{27}$$

$$b_3(\kappa)\xi_\kappa + [E_\kappa - \epsilon' + b_2(\kappa)]\eta_\kappa = 0. \tag{28}$$

Here the effective deformation amplitudes $b_2(\kappa)$ and $b_3(\kappa)$ are given by

$$b_2(\kappa) = \sqrt{\frac{5}{4\pi}}\,\beta_2\,x_2, \quad b_3(\kappa) = \sqrt{\frac{7}{4\pi}}\,\beta_3\,x_3. \tag{29}$$

The energy spectrum of deformed orbitals is obviously

$$E^{(\pm)}_\kappa = \frac{\epsilon+\epsilon'}{2} - b_2(\kappa) \pm \frac{1}{2}\sqrt{(\epsilon-\epsilon')^2 + 4b_3^2(\kappa)}. \tag{30}$$

The deformation parameters are found from eqs. (16) and (17),

$$\beta_L = \frac{x_L}{(2L+1)\omega_L}\,\rho_L, \tag{31}$$

where $x_2 = x^{(+)}_{jj} + {x'}^{(+)}_{j'j'}$ and $x_3 = 2y_{jj'}$. The density matrix (22) is now determined by the quantum numbers κ of the actually occupied pair of orbitals,

$$\rho_L(\kappa) = (-)^L\,\sqrt{4\pi(2L+1)}\,(-)^{j-\kappa}\begin{pmatrix} j & j & L \\ -\kappa & \kappa & 0 \end{pmatrix} z_L(\kappa), \tag{32}$$

where

$$z_2(\kappa) = \xi^2_\kappa + \eta^2_\kappa = 1, \quad z_3(\kappa) = 2\xi_\kappa\eta_\kappa, \tag{33}$$

and in the degenerate limit ($\epsilon = \epsilon'$) we have $|\xi_\kappa| = |\eta_\kappa| = 1/\sqrt{2},\ |z_3(\kappa)| = 1$. Due to time-reversal invariance, the same energy splitting (30) occurs for the orbitals with the opposite sign of projection κ.

F. Parity doublets

The single-particle intrinsic states $|\kappa)$ and $|-\kappa)$ found above, eq. (26), should be combined into intrinsic orbitals of certain parity,

$$|\psi_{\kappa;\pm}) = \frac{1}{\sqrt{2}}\Big[|\kappa) \pm (-)^{j-\kappa}|-\kappa)\Big]. \tag{34}$$

Since in the model each state $|\kappa)$ or $|-\kappa)$ is a combination of orbitals based on mixed levels j and j', in fact we have a quartet of relevant single-particle states or two parity doublets with the same $|\kappa|$. If the matrix element of the weak interaction between the single-particle spherical states $|jm)$ and $|j'm)$ equals w, its analog in the intrinsic frame connecting the partners of the doublets (34) is $w\xi_\kappa\eta_\kappa$. As it is clear from the symmetry arguments and seen from the set of equations (27,28), this product is proportional to the octupole effective deformation β_3 and the component ρ_3 of the single-particle density matrix. However, this quantity becomes a constant in the exceptional case of degenerate orbitals, eq. (32). Then the maximum value of the single-particle contribution of the weak interaction is, in this model, just $|w|/2$.

The Schiff moment operator (24) is responsible for the matrix element between two rotational states with the same spin I but opposite parities. This geometric matrix element gives, as follows also from general arguments [5, 14, 20],

$$\langle IM\kappa,\Pi|S_{10}|IM\kappa,-\Pi\rangle = -\frac{1}{\sqrt{\pi}}\,S^\circ\beta_2\beta_3\,\frac{M\kappa}{I(I+1)}. \tag{35}$$

The final answer (25) can be obtained multiplying the result (35) by $w\xi_\kappa\eta_\kappa/\Delta E_{I\kappa}$, where the energy denominator is given by the splitting of rotational partners of opposite parity. The collective enhancement for small frequencies of the even core is explicitly present in eq. (35). The energy splitting $\Delta E_{I\kappa}$ is determined mainly by the distance between the headbands of opposite parity that is of the order of the difference of phonon frequencies $\Delta\omega = |\omega_2-\omega_3|$. The effective moments of inertia of bands in the odd nucleus built on the parity doublets are expected to be close in heavy nuclei. For soft vibrations, $\Delta\omega$ gives another enhancement factor.

III. NUMERICAL DIAGONALIZATION OF THE MODEL

Here we show the results of the exact numerical solution of the two-level model based not on the assumption of preexisting soft phonons but on the full account of inter-particle interaction, including the primary interaction responsible for the existence of soft modes. We will be looking for the region of the parameter space that is favorable for the enhancement effects.

A. Nuclear Hamiltonian

We consider, as above in Sec. 2.5, the single-particle space of two spherical levels with the same $j=j'$ and opposite parity; their spherical energies are taken as $\epsilon_j = 0$ and $\epsilon_{j'} = \epsilon$. The dynamics in the particle-particle channel can be expressed in terms of the pair operators from the same j-level,

$$P_{LM} = \frac{1}{\sqrt{2}}\sum_{mm'} C^{LM}_{jm\,jm'}\,a_{jm'}a_{jm}, \quad P'_{LM} = \frac{1}{\sqrt{2}}\sum_{mm'} C^{LM}_{jm\,jm'}\,a_{j'm'}a_{j'm}, \tag{36}$$

where only even total momenta, $L=0,...,2j-1$, are allowed, and the pair operator changing parity of the state,

$$R_{LM} = \sum_{mm'} C^{LM}_{jm'\,jm}\,a_{jm}a_{j'm'}, \tag{37}$$

where all values of the pair spin, $L=0,1,...,2j$, are possible. The most general two-body Hamiltonian,

$$H_{\rm int} = H_{jj} + H_{j'j'} + H_{jj'} + V, \tag{38}$$

includes the interactions inside each j-level,

$$H_{jj} = \sum_{LM} h_L P^\dagger_{LM}P_{LM}, \quad H_{j'j'} = \sum_{LM} h'_L {P'_{LM}}^\dagger P'_{LM}, \tag{39}$$

the pair transfer between the levels,

$$H_{jj'} = \sum_{LM} g_L \Big(P^{\dagger}_{LM} P'_{LM} + {P'_{LM}}^{\dagger} P_{LM} \Big), \tag{40}$$

and, finally, scattering of the mixed pairs,

$$V = \frac{1}{4} \sum_{LM} V_L R^{\dagger}_{LM} R_{LM}. \tag{41}$$

We specify the model choosing only the interactions associated with the collective dynamics: pairing part $G > 0$,

$$h_0 = h'_0 = g_0 = -G; \tag{42}$$

quadrupole-quadrupole interaction in the particle-hole channel that, after the angular momentum recoupling, corresponds to

$$h_L = h'_L = 5\varkappa_2 \left\{ \begin{matrix} j & j & 2 \\ j & j & L \end{matrix} \right\}; \tag{43}$$

and octupole-octupole interaction that similarly gives rise to

$$V_L = 7\varkappa_3 \left\{ \begin{matrix} j & j & 3 \\ j & j & L \end{matrix} \right\}. \tag{44}$$

Thus, the model Hamiltonian is characterized by four parameters, ϵ, G, $\varkappa_2$ and $\varkappa_3$. Attractive forces correspond to positive G, $\varkappa_2$ and $\varkappa_3$.

Also useful are the operators in the particle-hole channel,

$$Q^{\dagger}_{\lambda\mu}(j_1 j_2) = \sum_{m_1 m_2} (-)^{j_1 - m_1} \begin{pmatrix} j_1 & \lambda & j_2 \\ -m_1 & \mu & m_2 \end{pmatrix} a^{\dagger}_{j_1 m_1} a_{j_2 m_2}, \tag{45}$$

for different angular momenta λ and all combinations of j_1 and j_2. These operators have a symmetry property

$$Q^{\dagger}_{\lambda\mu}(j_1 j_2) = (-)^{j_1 - j_2 + \mu} Q_{\lambda -\mu}(j_2 j_1). \tag{46}$$

In these terms, our multipole-multipole interactions are

$$H^{(2)} = -\frac{5\varkappa_2}{2} \sum_{\mu} \Big[Q^{\dagger}_{2\mu}(jj) Q_{2\mu}(jj) + Q^{\dagger}_{2\mu}(j'j') Q_{2\mu}(j'j') \Big] \tag{47}$$

and

$$H^{(3)} = -\frac{7\varkappa_3}{2} \sum_{\mu} \Big[Q^{\dagger}_{3\mu}(j'j) Q_{3\mu}(j'j) + Q^{\dagger}_{3\mu}(jj') Q_{3\mu}(jj') \Big]. \tag{48}$$

The Schiff moment operator is given by

$$S_{\mu} = -\sqrt{2j+1}\, s \Big[Q_{1\mu}(j'j) + Q_{1\mu}(jj') \Big], \tag{49}$$

while the weak interaction,

$$W = \sqrt{2j+1}\, w \Big[Q_{00}(j'j) + Q_{00}(jj') \Big], \tag{50}$$

is characterized by one scalar w for the transition between the states $|jm)$ and $|j'm)$. As we are interested in the trends of the expectation values of the Schiff moment in a function of nuclear forces, the values of the coefficients s and w are irrelevant. Below we set $w = 1$ and $(j'm = j|S_{\mu=0}|jm = j) = \sqrt{j/(j+1)}$.

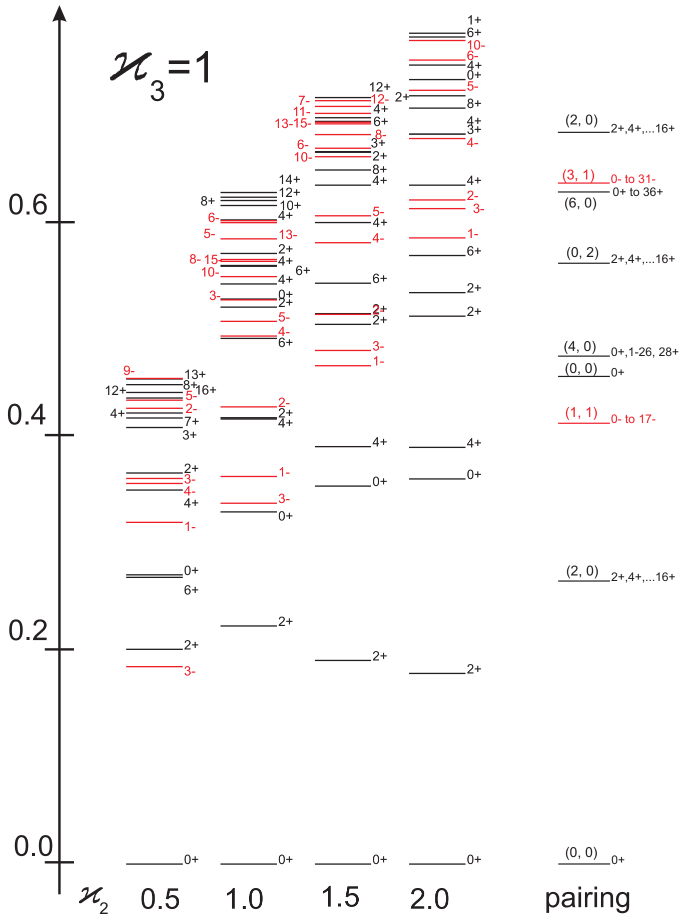

Figure 1: The spectra of the 6-particle system for $\epsilon = 0.2$ and $G = 0.2$. For the left four spectra, a fixed value of the octupole strength, $\varkappa_3 = 1.0$, and a variable quadrupole interaction parameter, $\varkappa_2$=0.5, 1, 1.5 and 2, are used. The most right spectrum corresponds to the pairing Hamiltonian, $\varkappa_2 = \varkappa_3 = 0$, where seniorities $(s_j,\, s_{j'})$ are also marked. The negative parity states are shown in red.

B. Numerical results

Fig. 1 shows the results for the energy spectrum obtained in the exact diagonalization of the strong Hamiltonian for 6 particles on two levels with $j = j' = 17/2$. Here we fix the octupole strength $\varkappa_3 = 1$ and the pairing strength equal to the energy spacing between the single-particle levels, $\epsilon = G = 0.2$.

In the right column we show for comparison the spectrum for the pure pairing interaction, $\varkappa_2 = \varkappa_3 = 0$. As well known from the analysis of the exact solution of the pairing problem [31], partial seniority quantum numbers (or quasispins) s_j are conserved, and every eigenstate is characterized, apart from the angular momentum quantum numbers IM, by the seniorities $s_j, s_{j'}$. The states with nonzero seniority are multiple degenerate with respect to total spin. The states with the odd seniority $s_{j'}$ have negative parity. The degenerate states with $s_j = 2, s_{j'} = 0$ show a clear pairing energy gap that exceeds the single-particle spacing ϵ.

The first four columns show spectra in the presence of multipole-multipole interactions for $\varkappa_3 = 1$ and different values of $\varkappa_2$. The quadrupole collective state 2^+ emerges within the pairing gap with energy only weakly changing as a function of the quadrupole constant. At relatively weak quadrupole strength, the collective low-lying 3^- state is also present. However, as a consequence of our limited single-particle space, the octupole and quadrupole branches essentially compete because, due to their opposite parity, they require very different distortion (polarization) of the quasiparticle vacuum.

The situation is different in the neighboring odd system ($N = 7$), Fig. 2, where the same Hamiltonian parameters are used. In the case of the pairing only, we have two "vacuum" states with opposite parity and the same spin 17/2 which correspond to a position of the odd particle on the j-level or on the j'-level. This asymmetry sets into action the mechanisms qualitatively described in Sec. 2. We see low-energy collective excitations, which, in the region of approximately equal strength of quadrupole and octupole branches, create parity doublets $(17/2^+, 17/2^-)$. Their

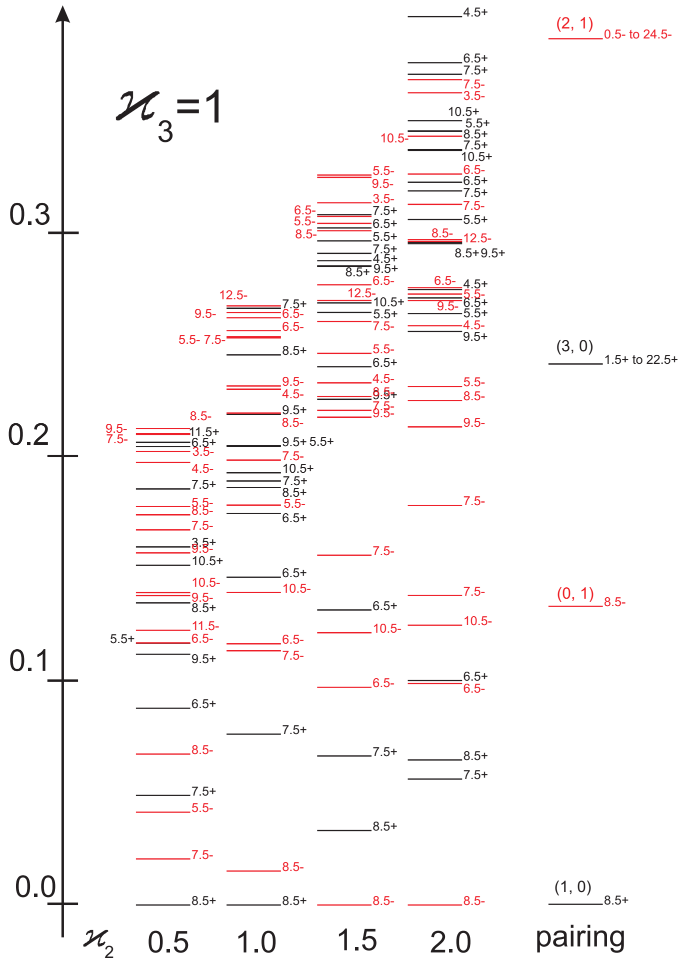

Figure 2: Same as Fig. 1 but for a 7-particle system.

minimum energy splitting, 0.15 at $\varkappa_2 = \varkappa_3 = 1$, is smaller than the single-particle spacing.

C. Degenerate case

In the model with $j = j'$, the interactions are symmetric with respect to the interchange $\mathcal{I} : (j \leftrightarrow j')$ of levels of opposite parity. This operation commutes with spatial inversion in an even system and anticommutes in the odd one, $\mathcal{P}\mathcal{I} = (-)^N \mathcal{I}\mathcal{P}$, where N is the number of particles. For degenerate levels ($\epsilon = 0$), $\mathcal{I}$ becomes the symmetry of the strong Hamiltonian. But for an odd system, $\mathcal{I}$-symmetry is incompatible with parity. Since the full $\mathcal{I}$-symmetry is accidental, we still classify the nuclear eigenstates by parity Π but in this case two states of opposite parity are exactly degenerate being related by the $\mathcal{I}$-operation. Thus, in the odd system we have exact parity doublets, and all many-body states are pairwise degenerate. In the even system, $\mathcal{P}$ and $\mathcal{I}$ have common eigenstates with corresponding values ± 1.

In our definitions, both the weak interaction W and the Schiff moment operator $\mathbf{S}$ change parity but preserve $\mathcal{I}$-symmetry. The transition matrix elements of $\mathbf{S}$ in the even nucleus occur only within the class of states with the same $\mathcal{I}$. In the odd case we classify the stationary states (with no weak interaction) by parity so that the new symmetry places no constraints onto matrix elements of $\mathbf{S}$.

The spectrum of the exceptional case, $\epsilon = 0$, is shown in Fig. 3 for $N = 6$. In the pure pairing model (the right column), the well known spin-degenerate seniority spectrum ($s = s_j + s_{j'}$) is given by

$$E(s) = -\frac{G}{2(2j+1)}(N-s)(4j+4-N-s), \tag{51}$$

where even values of the seniority quantum number $s \neq 0$ increase energy through the Pauli blocking effect on

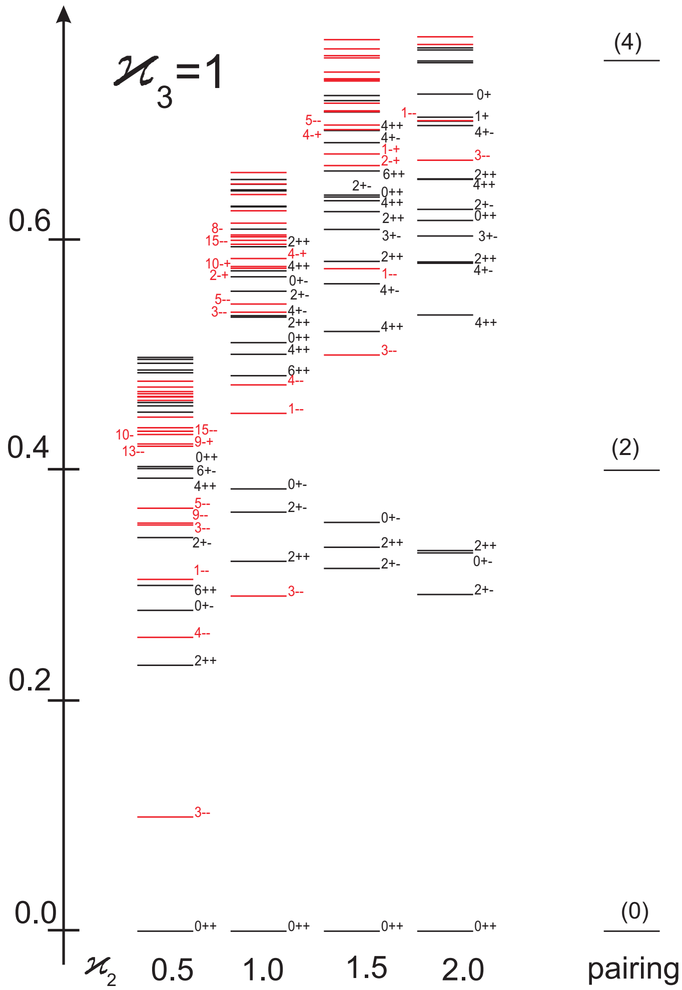

Figure 3: The spectra of the 6-particle system with degenerate single particle levels $\epsilon = 0$; $G = 0.2$ and $\varkappa_3 = 1.0$. The set of values $\varkappa_2$=0.5, 1, 1.5 and 2 is used. The pure pairing spectrum, $\varkappa_2 = \varkappa_3 = 0$, with total seniority marked is to the right. Most of the lowest states are labeled as $J^{\mathcal{PI}}$. The negative parity states are shown in red.

quenched pairing. The states for non-zero multipole-multipole forces are labeled by quantum numbers $\Pi\mathcal{I}$. The situation with the lowest collective states inside the gap is however not significantly different from that observed for $\epsilon \neq 0$. Again as $\varkappa_2$ grows, we see the *destructive* influence of the quadrupole mode onto the octupole mode; the latter is strongly pushed up in energy. In our analytical consideration, Sec. 2.1, the interplay of the quadrupole and octupole modes was *constructive* (and this is what is seen in global systematics and in xenon isotopes [24]). It follows from eq. (4) that the mutually supportive interaction of the modes comes from the three-phonon ahnarmonicity, while the conventional Hamiltonian of the type (38) makes the coexistence of the modes less probable, at least in the truncated orbital space. We need to mention the crossing of the lowest 2^{++} and 2^{+-} levels at $\varkappa_2 = 1.27$; then the matrix element of the Schiff moment between the lowest states 2^{+-} and 3^{--} does not vanish, in contrast to the matrix element between 2^{++} and 3^{--}.

D. Schiff moment

Fig. 4 shows the results for the matrix elements of the Schiff moment (in the even and in the odd systems) and of the weak interaction (in the odd system). In the even case (the left column, $N = 6$), the Schiff moment (the reduced matrix element between the lowest "phonon" states 2^+ and 3^- shown in the upper left panel) strongly depends on the single-particle spacing which was partly discussed above. For all values of ϵ, the maximum of this matrix element is reached in the region of approximately equal strength $\varkappa_2$ and $\varkappa_3$.

The three remaining panels on the left show the excitation energies of the lowest 2^+ and 3^- states for different

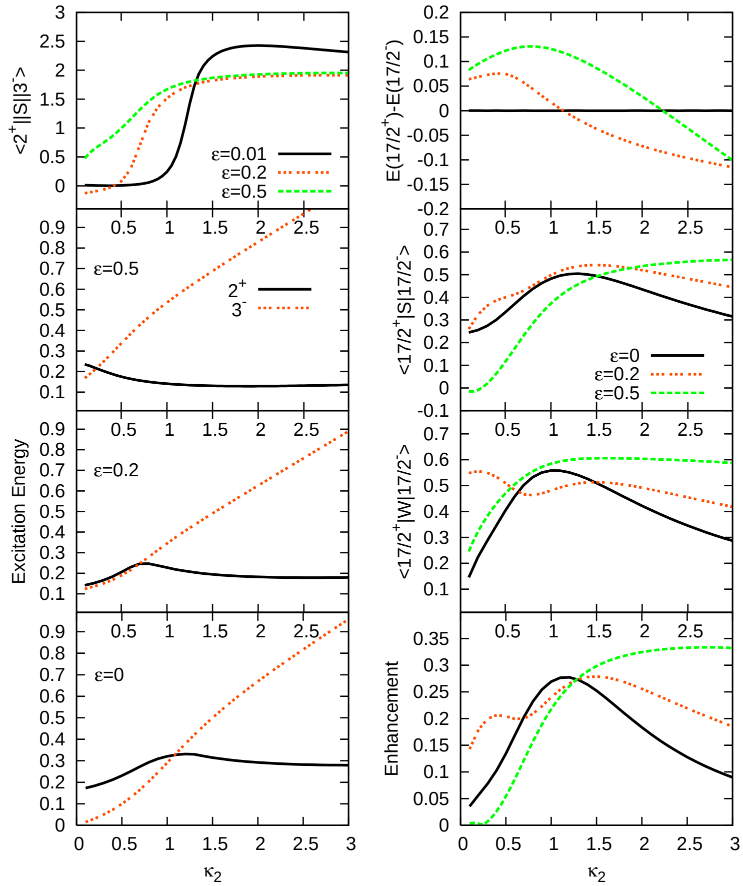

Figure 4: The system of two $j = 17/2$ levels is studied as a function of quadrupole interaction strength $\varkappa_2$ at fixed values $\varkappa_3 = 1$ and $G = 0.2$. Three cases of single-particle splitting are considered: $\epsilon = 0$ (or very small value of 0.01 to remove abrupt numerical discontinuities), 0.2 and 0.5. The left column is for the $N = 6$ particle system. Three lower left panels show the excitation energies of 2^+ and 3^- levels for different ϵ as labeled. The top left plot shows the reduced matrix element of the Schiff operator between these states. The 7-particle system is depicted in the right column plots. The splitting of the ground state doublet is on the right top followed below by the plots of expectation values of the Schiff operator, weak matrix element and their product. Three curves, solid (black), dotted (red) and dashed (green), correspond to the same set of single-particle spacings $\epsilon = 0$, 0.2 and 0.5, respectively.

single-particle spacings ϵ. As ϵ and $\varkappa_2$ increase (at fixed $\varkappa_3$), the destructive interaction of the modes pushes the octupole phonon energy to high energy. However, at the reasonable value $\epsilon = 0.2$ that corresponds to the spectra shown earlier, there is a region, where $\varkappa_2$ and $\varkappa_3$ are of the same order and both resulting phonon frequencies are low.

The right column of Fig. 4 gives the results for the odd system, $N = 7$, as a function of $\varkappa_2$. The upper panel shows the splitting of the parity doublet $E(17/2^+) - E(17/2^-)$. Both matrix elements, of the Schiff moment and of the weak interaction, show a well pronounced maximum at $\varkappa_2 \sim \varkappa_3 \sim 1$ for not very large single-particle spacing ϵ. This is exactly what was the purpose of the study. Of course, the precisely degenerate case, $\epsilon = 0$, is unphysical (in order to justify perturbation theory (25), the actual calculation here assumed a very small spacing still exceeding the off-diagonal matrix element of the weak interaction). However, a noticeable effect is present in the case of $\epsilon = 0.2$ as well.

IV. CONCLUSION

We discussed the arguments in favor of the hypotheses of possible enhancement of the nuclear Schiff moment, and therefore of the effects of $\mathcal{P}, \mathcal{T}$-violating weak interactions, in nuclei with the simultaneous presence of soft collective modes of quadrupole and octupole nature. If this idea is correct, the pool of possible nuclei − candidates for the successful search of the atomic EDM − would significantly broaden.

In our analytical model, we showed that in the odd neighbor of the even spherical nucleus with soft vibrational

modes the unpaired particle leads to the spontaneously broken rotational symmetry. The arising effective deformation can be described as a condensate of phonons. The strength of the condensate is inversely proportional to the small phonon frequencies in the even nucleus. This leads to the enhancement of the intrinsic Schiff moment, in analogy to what was known for nuclei with static quadrupole and octupole deformation. As a result, we obtain the enhancement of the Schiff moment in the laboratory frame that emerges due to the $\mathcal{P}, \mathcal{T}$-violating weak interaction, whose discovery is the primary goal of experimental and theoretical research in this area.

The exact numerical study of a similar two-level model confirms the existence of the region in the parameter space (single-particle spectrum and the strengths of pairing and multipole-multipole interactions) where the low-lying quadrupole and octupole modes coexist, and where matrix elements of the weak interaction and of the Schiff moment are indeed enhanced. The exact calculation does not introduce any intrinsic frame and fully preserves rotational symmetry and (in the absence of the weak interaction) parity of stationary states. Although the model studied above had a limited single-particle space and a small number of valence particles that precludes the appearance of very strong collectivity, the presence of the enhancement is visible.

We pointed out the difference between the analytical consideration and the numerical model in the character of the interaction between the quadrupole and octupole modes. The numerical study, being exact in the framework of the two-level model, assumed the conventional two-body Hamiltonian. Then the coexistence of the modes of incompatible symmetry is suppressed by their destructive competition for the available supply of single-particle excitations. The analytical model assumed the strong anharmonic interaction between the modes that leads to their mutual support and the appearance of the quadrupole condensate in the state of the even nucleus with one octupole phonon. Such cubic anharmonicities are rather weak if considered in the next order of the random phase approximation built on the two-body multipole-multipole interaction. However, currently there is a broad discussion of the role of three-body forces, see for example [32], in the nuclear structure beyond light nuclei. The possible collective effects of three-body forces (in this respect it does not really matter, bare or effectively induced in nuclear matter) were briefly discussed, in relation to various physical phenomena in nuclear physics, in [33]. One of the main new effects is the emergence of three-phonon anharmonicity. The predicted positive correlation of quadrupole and octupole modes is well seen in the chain of xenon isotopes [24]. Such studies can be important in many questions of nuclear structure, independently of the problem connected with weak interactions.

V. ACKNOWLEDGMENTS

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